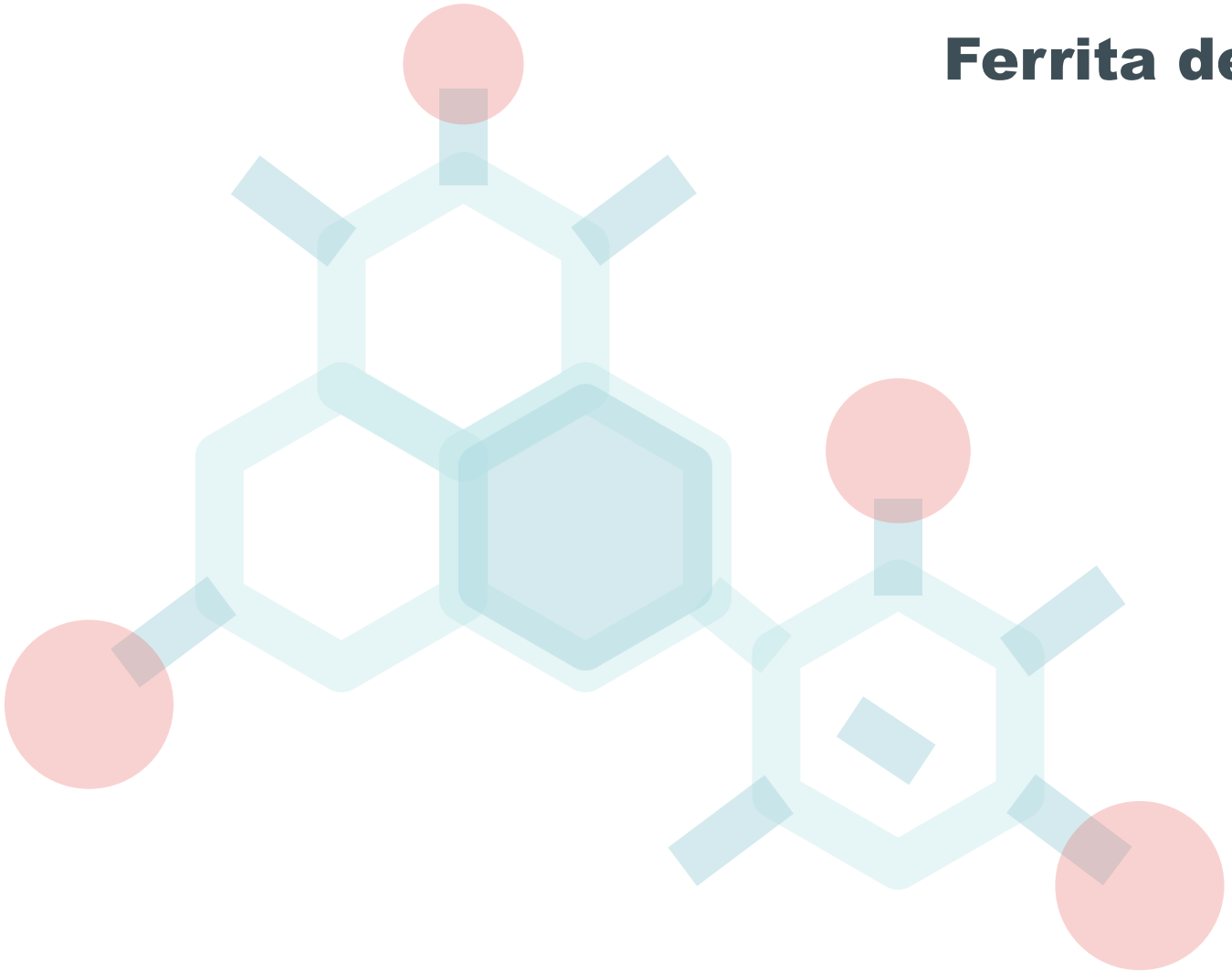
Cálculos de Estructura Electrónica en Perovskitas
Ferrita de Bismuto y Cromita de Itrio

MSc. Shigueru Nagata



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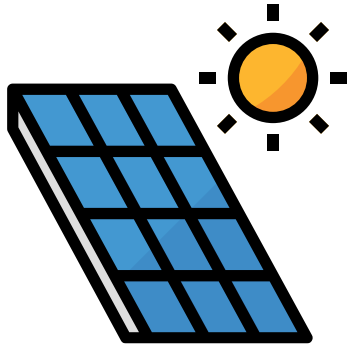
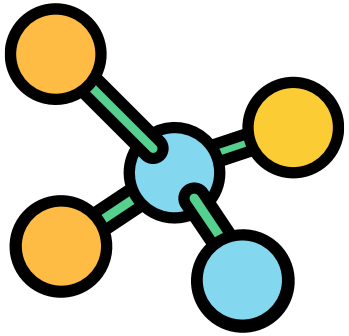


Panel Solar

Silicio



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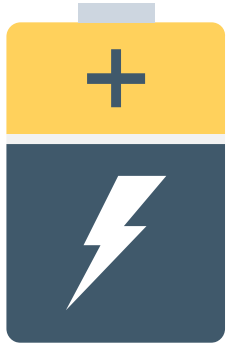
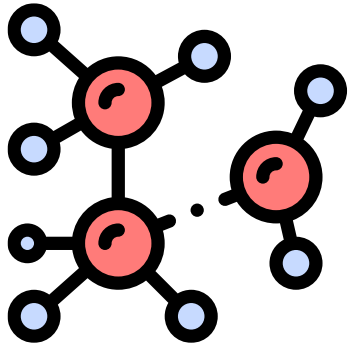
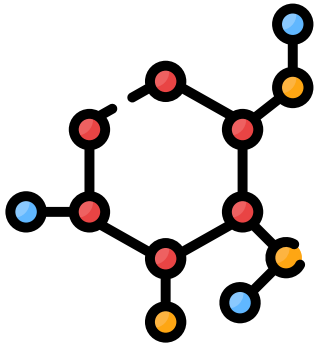




Litio

Disco Duro

Vanadio



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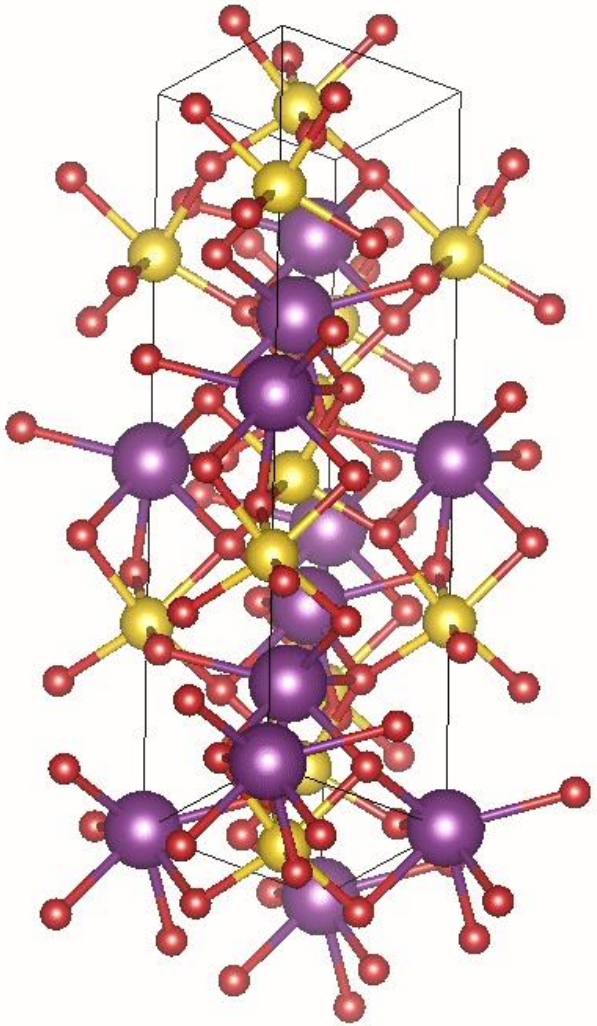

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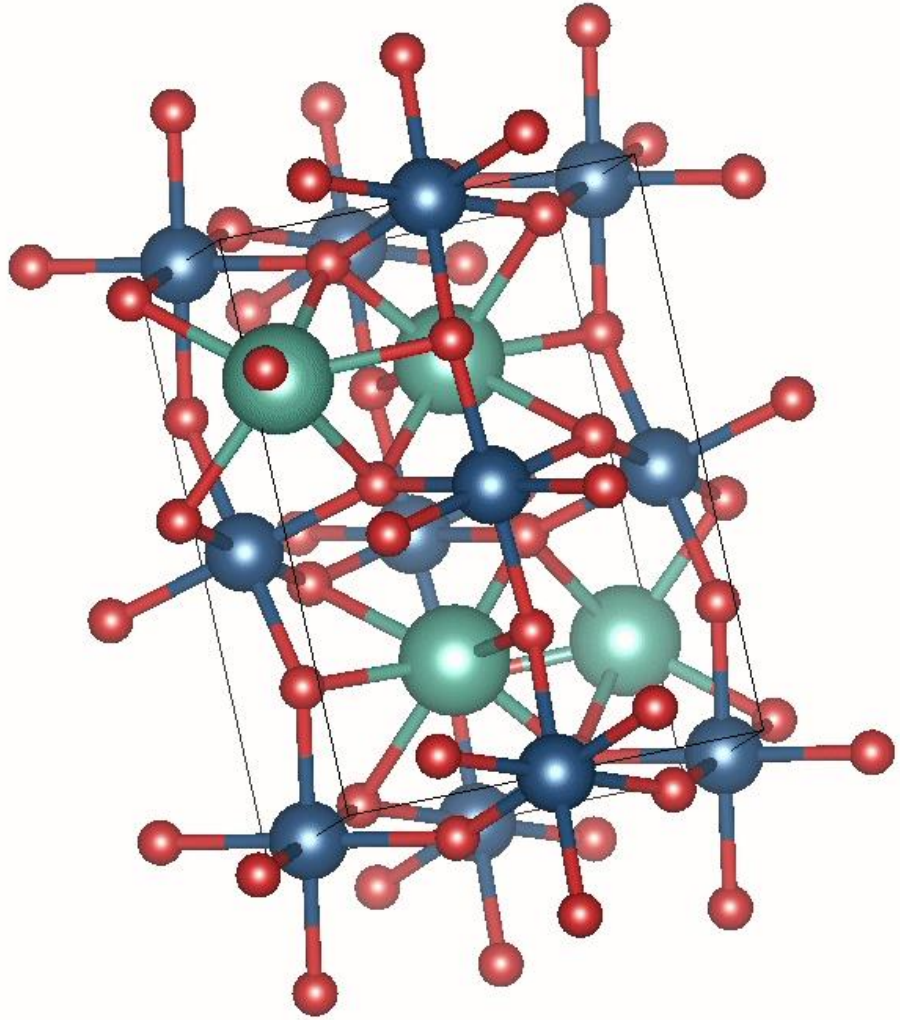
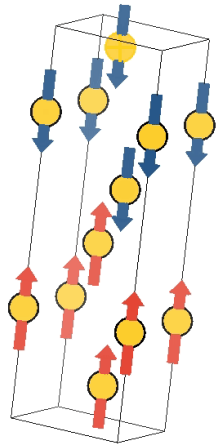
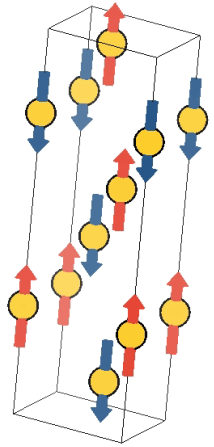


Ferrita de Bismuto

Arreglos Antiferromagnéticos



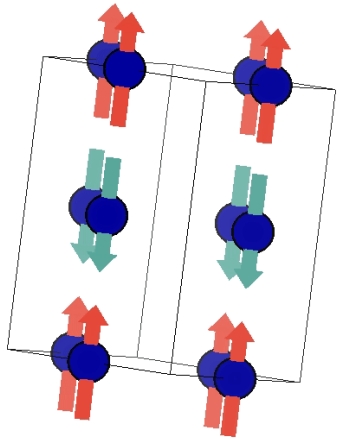
Tipo A



Tipo G

Cromita de Itrio

Arreglos Antiferromagnéticos



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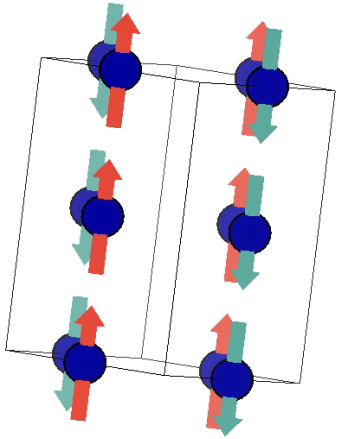

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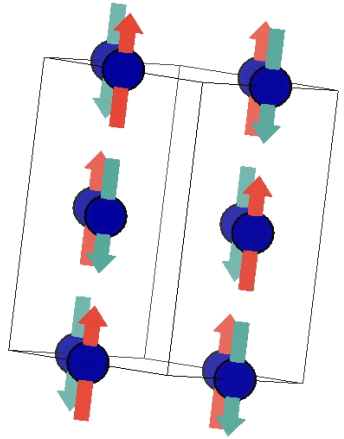


Tipo G

Banda de Conducción
Gap de Energía
Banda de Valencia

Banda de Conducción
Conductor
Banda de Valencia

Banda de Conducción
Semiconductor
Banda de Valencia

Banda de Conducción
Aislante
Banda de Valencia

Teoría del Funcional de Densidad

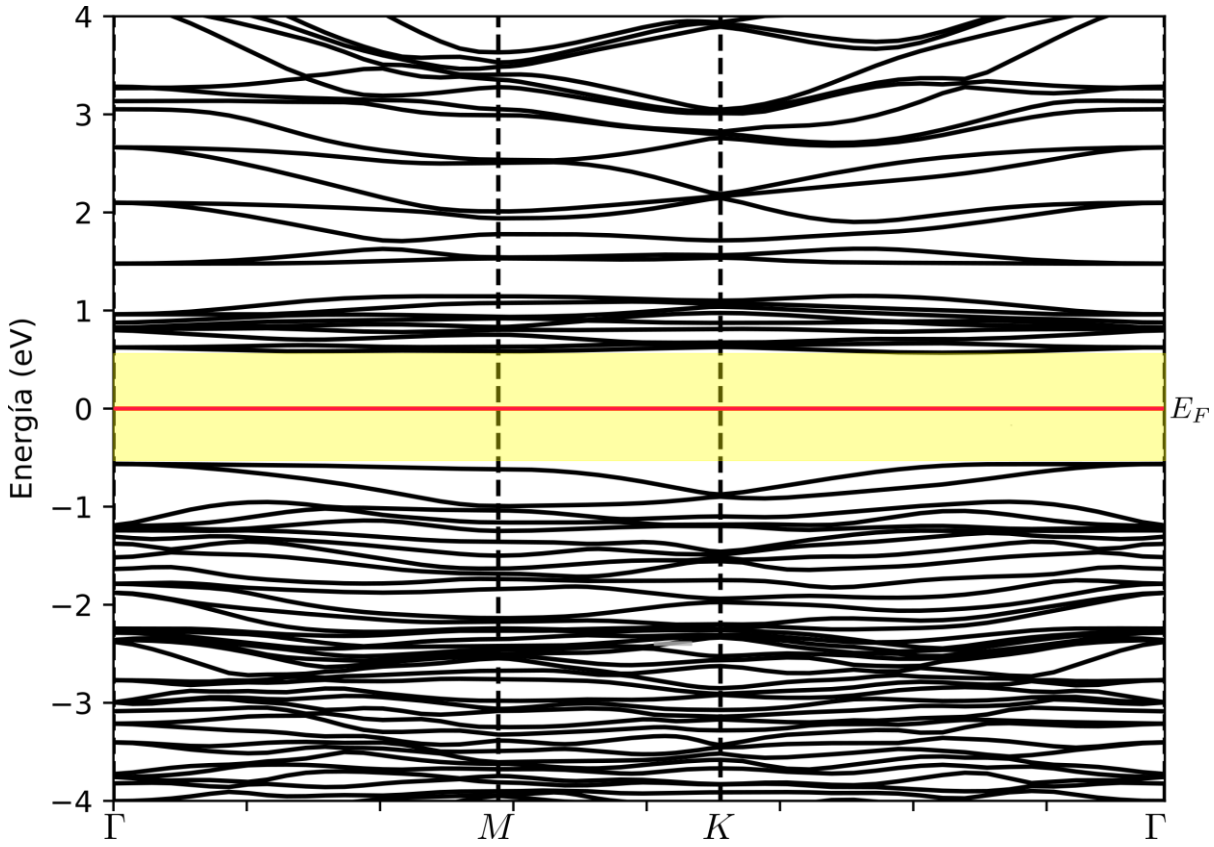
Solución de

Ecuación de Schrodinger

Aproximaciones

Born-Oppenheimer	Teoremas de Hohemberg-Kohn
Nucleos atómicos fijos en el espacio	Electrones como densidad de carga

Ferrita de Bismuto



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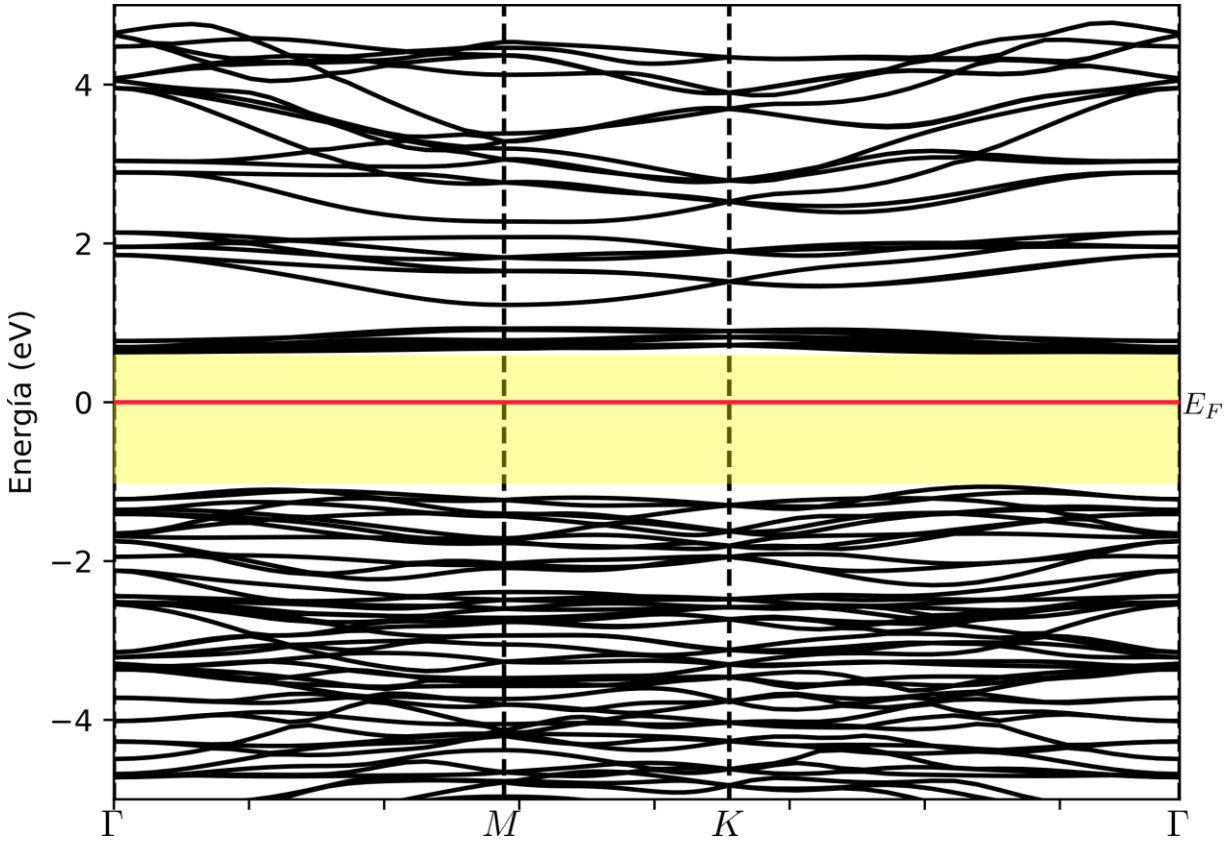

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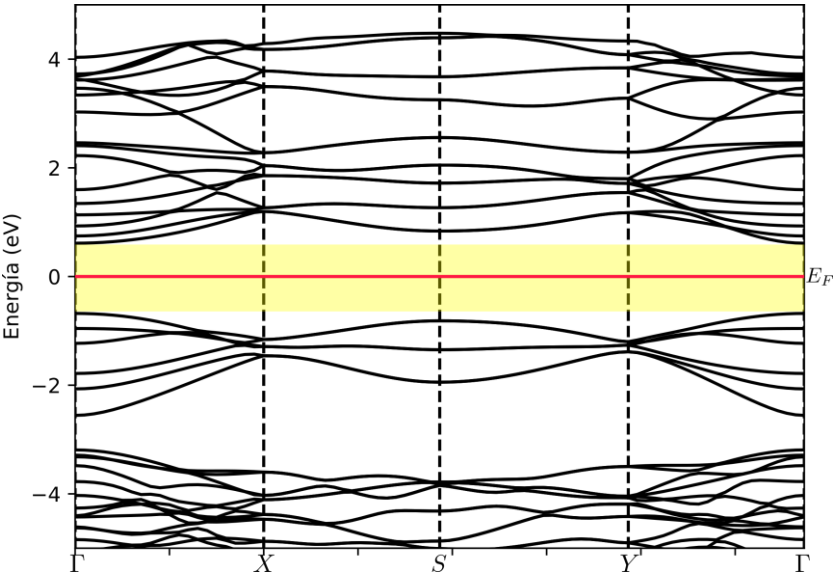

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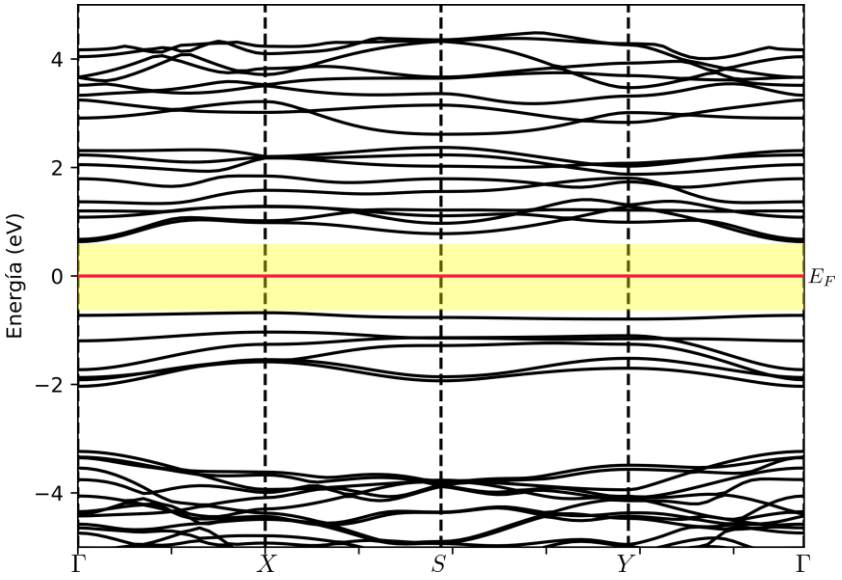

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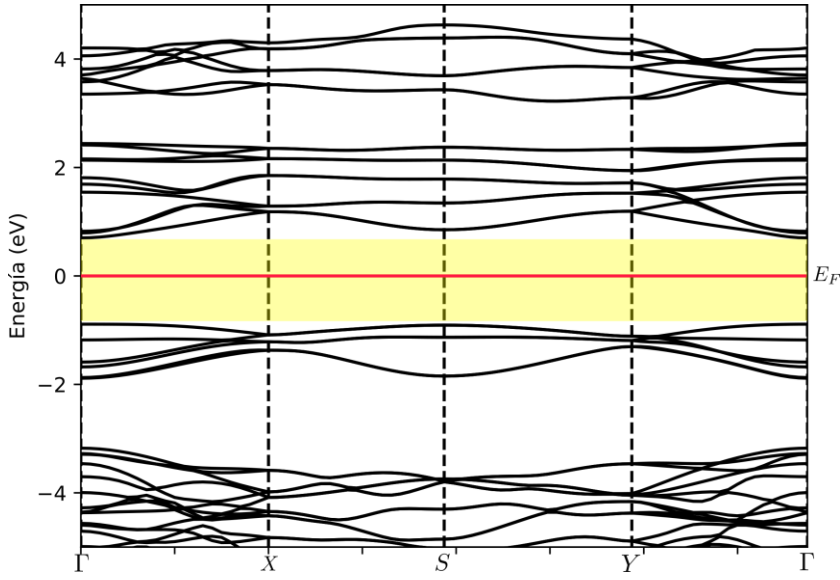
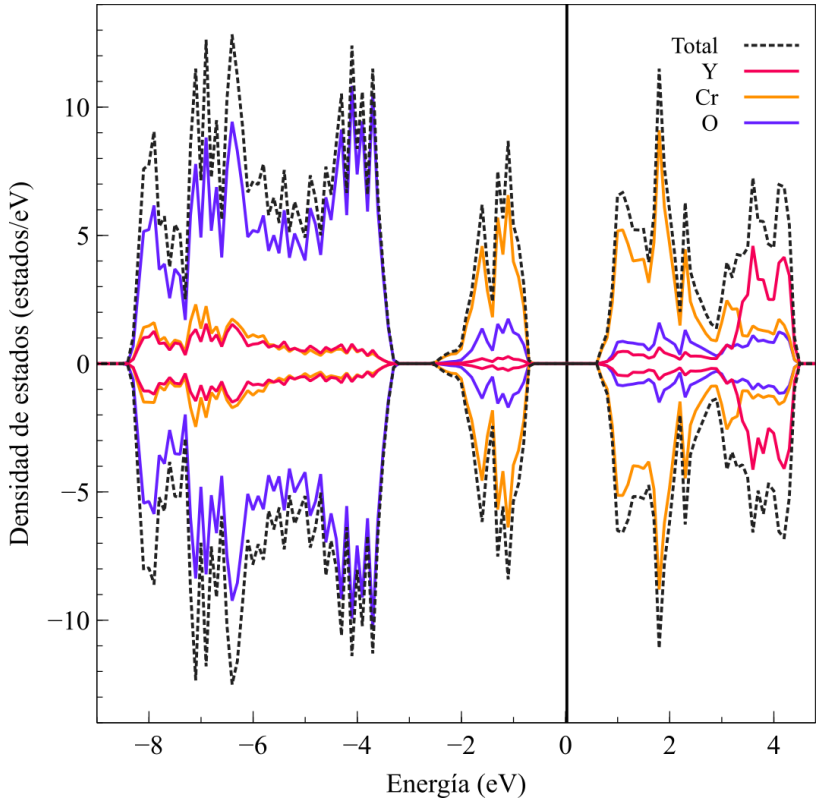


Arreglo Tipo G

Cromita de Itrio



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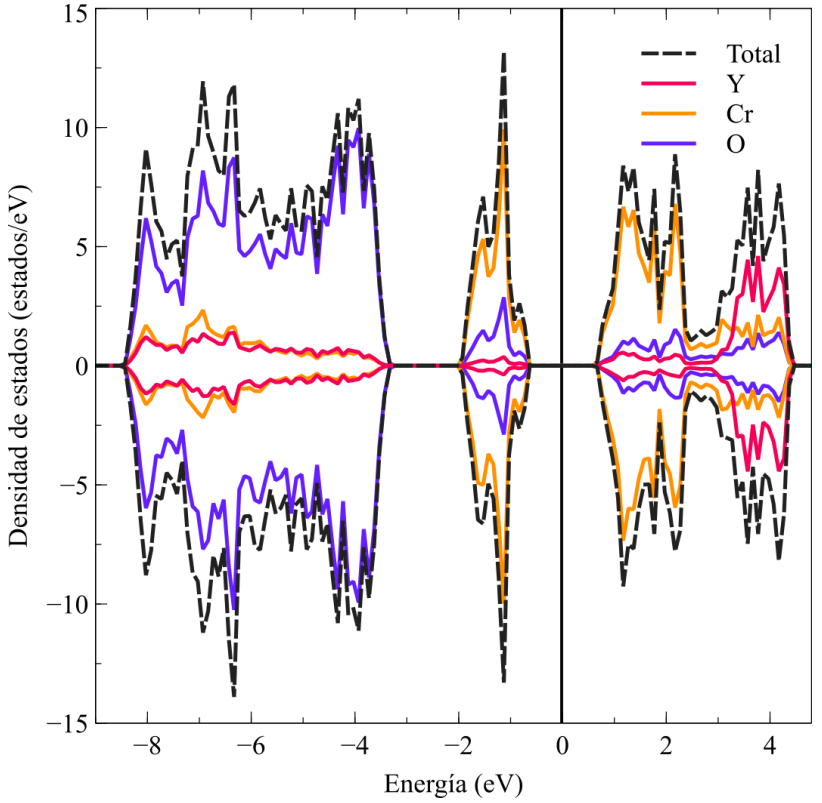

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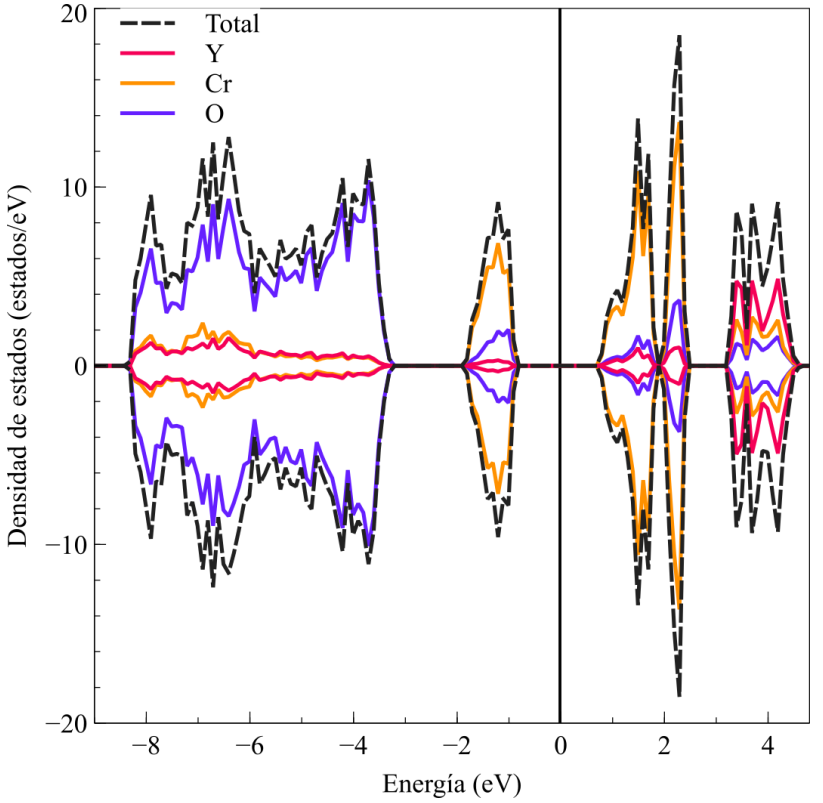

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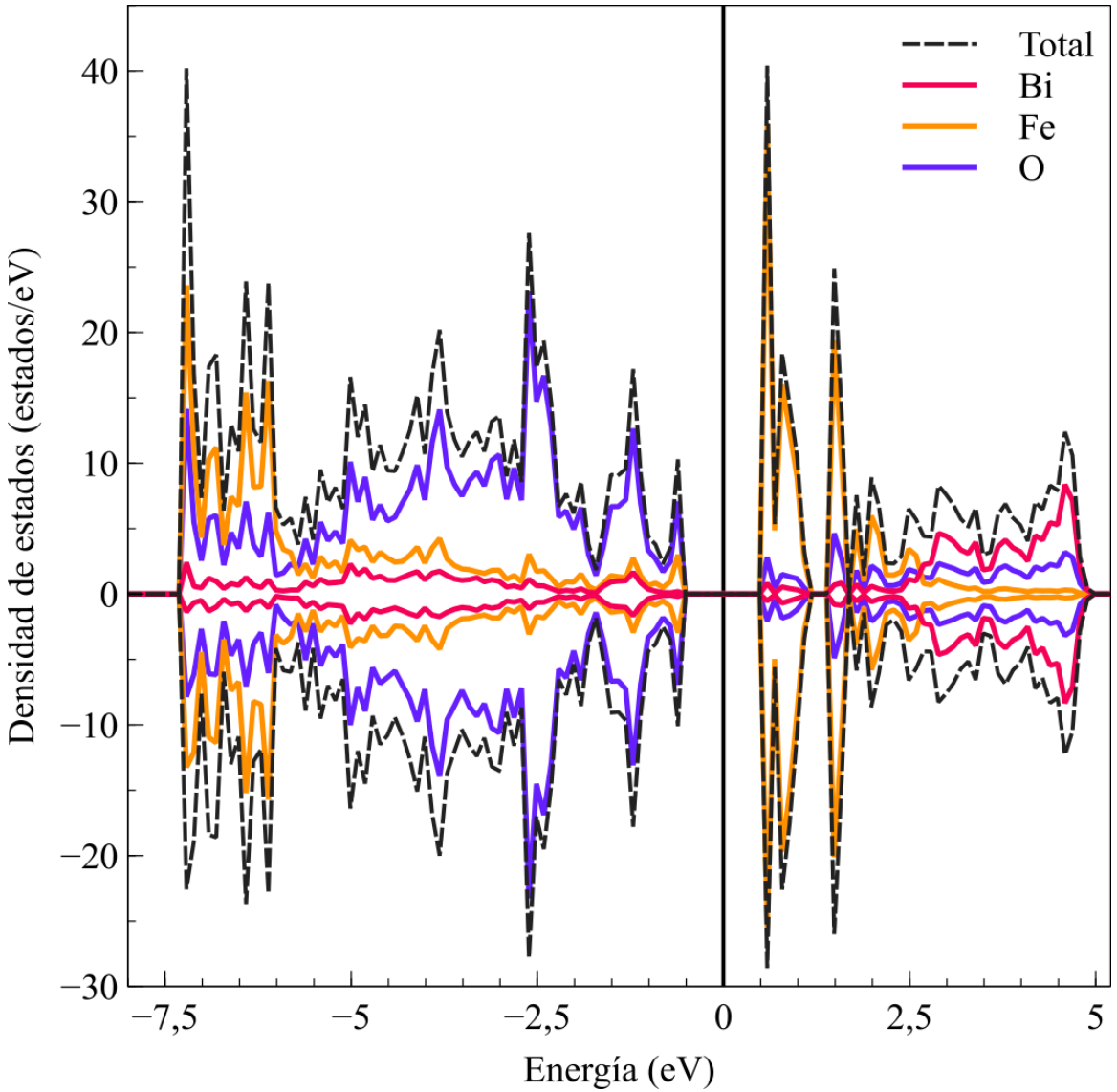
Ferrita de Bismuto



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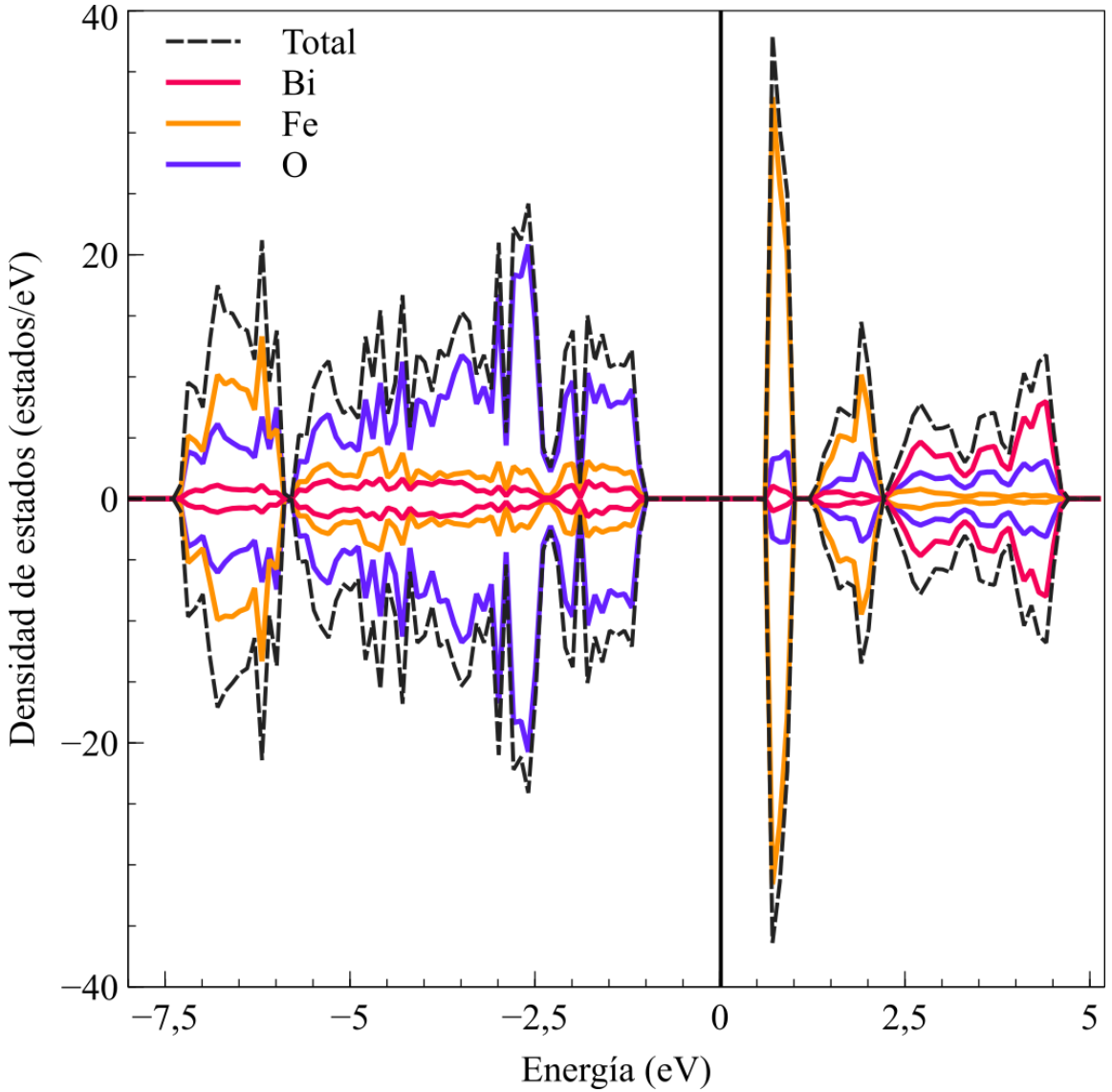

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